

Pentyl 2-hydroxypropanoate
6382-06-5 | DTXSID70858752

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: $1.31\text{e-}11$ cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: $4.90\text{e-}01$

Confidence level: $8.53\text{e-}01$

Nearest Neighbors from the Training Set

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2-Ethoxyethyl isobutyrate

Measured: $1.35\text{e-}11$

Predicted: $1.28\text{e-}11$

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Ethyl 3-ethoxypropionate

Measured: $2.29\text{e-}11$

Predicted: $1.63\text{e-}11$

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Butyl butyrate

Measured: $1.06\text{e-}11$

Predicted: $1.06\text{e-}11$

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Bornyl acetate

Measured: $1.39\text{e-}11$

Predicted: $1.36\text{e-}11$

Image not found

Pentyl acetate

Measured: $7.55\text{e-}12$

Predicted: $6.38\text{e-}12$